SCIT — UKRAINIAN SUPERCOMPUTER PROJECT

Valeriy Koval, Sergey Ryabchun, Volodymyr Savyak,
Ivan Sergienko, Anatoliy Yakuba

Abstract: The paper describes a first supercomputer cluster project in Ukraine, its hardware, software and characteristics. The paper shows the performance results received on systems that were built. There are also shortly described software packages made by cluster users that have already made a return of investments into a cluster project.

Keywords: supercomputer, cluster, computer structure.

ACM Classification Keywords: C.5.1 Super computers, C.1.4 Parallel Architectures.

Introduction

To solve the most important tasks of an economy, technology, defense of Ukraine, that have large and giant computing dimensions, we need to be able to calculate extralarge information arrays. Such extremely large computations are impossible without modern high-performance supercomputers.

Unfortunately, such computational resources are almost unavailable in Ukraine today. This can cause a precarious situation development in a different country's life areas. We can lose leading positions in a science, science intensive products' development, complex objects and processes modeling and design technologies.

It is also impossible to import large supercomputers for the above mentioned tasks, because of embargo (for really powerful supercomputers), their extra-large prices, practically impossible upgrade, requirements to control the usage of imported supercomputers from abroad. In this situation Ukraine and other countries (India, China, Russia, Belarus) need to design its national supercomputers [1].

Today in Glushkov Institute of Cybernetics NAS of Ukraine, two high-performance and highly effective computational cluster systems SCIT-1 and SCIT-2 are running in an operation-testing mode. They are built on the basis of modern microprocessors INTEL® XEON™ и INTEL® ITANIUM® 2.

On the basis of these supercomputer systems, a powerful joint computer resource will be built. It will be available for access for users from different organisations from different regions from all the NAS of Ukraine. The systems built are focused to applications from the fields of molecular biology, genetics, science of materials, solid-state physics, nuclear physics, semiconductor physics, astronomy, geology.

Development Ideology

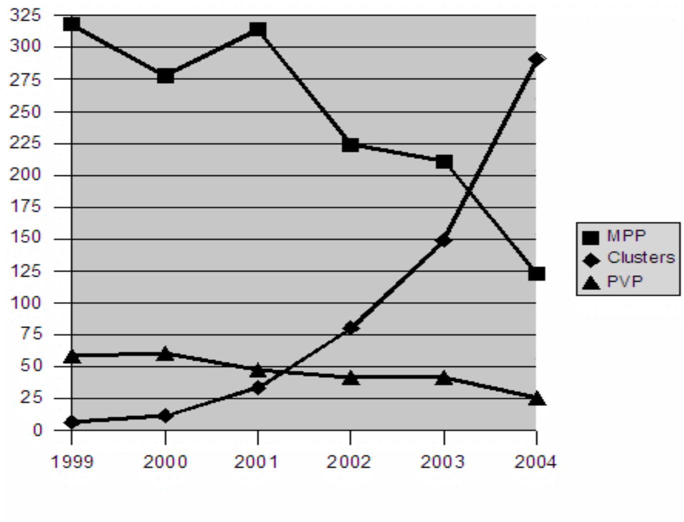
While developing a supercomputer, system scientists and engineers face, a great amount of questions that requires to run a different kind of experiments. The experiments are run to understand a performance, features and characteristics of architecture, hardware platform for computing node solution, node interconnections, networking interfaces, storage system [2].

To make a right decision on system architecture we have made an analysis of world supercomputer tendencies. One of major sources we used was top500 list of the largest supercomputer installations. An analysis we made proves us, that a solution of cluster architecture is a right one.

Cluster computer system – is a group of standard hardware and software components, coupled to solve tasks. Standard single processor or SMP (symmetric multiprocessor system) are used as processing elements in a cluster. Standard high-performance interconnect interfaces (Ethernet, Myrinet, SCI, Infiniband, Quadrics) are used to connect processing elements in a cluster system.

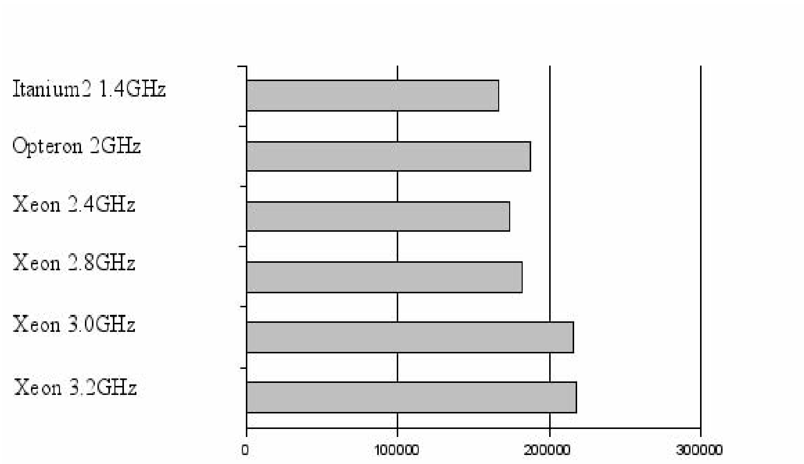
A development of supercomputer systems with cluster architecture is one of the most perspective ways in the world of high-performance computations today. The amount of supercomputer clusters installed in the world in increasing rapidly and the amount of finances spent for this direction is also increased.

Tendencies of a development of supercomputers in the world for MPP (Massively Parallel Processing), PVP (Parallel Vector Processor) and cluster systems are shown on a Picture 1. As shown on the picture below, clusters are dominated in top500 list. For the several last years, an amount of cluster systems in the list have grown and an amount of MPP and PVP systems is going down.



Picture 1. World supercomputer tendencies

When making a selection of a hardware platform of computational nodes we analyzed price/performance ratio. As LINPACK is rather narrow test, we choose SPECfp tests understand a performance of nodes on the basis of different kind of real applications. The prices we calculated were taken from Ukrainian IT market operators. The diagram received in analysis is shown on a Picture 2.

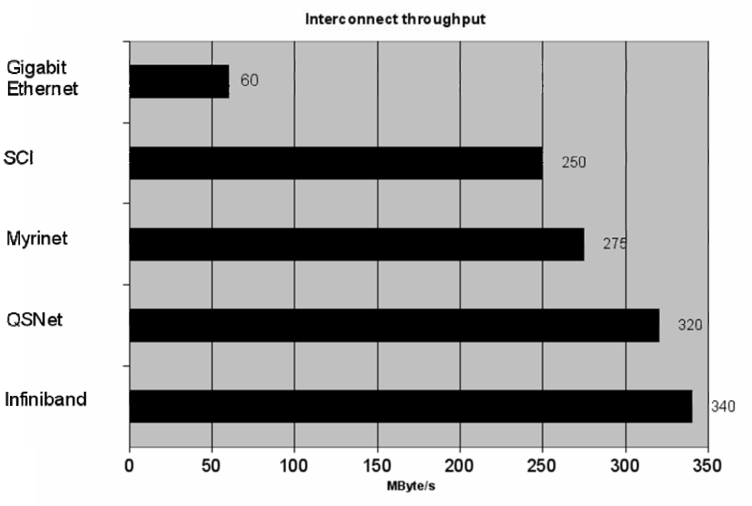


Picture 2. Price/performance ratio on the basis of SPECfp analysis

Today also new SPEChpc tests are available, that can give us an understanding of hpc computers performance for an applications from chemical, environment, seismic area and also OpenMP and MPI applications testing.

Price/performance analysis is made with a calculation of costs of all the main components of a system and its environment with a focus on a theoretical peak 300 GFlops performance, which is near 120 000 SPECfp. We have also take into consideration performance downsize for different platforms scaling on the basis of self made tests.

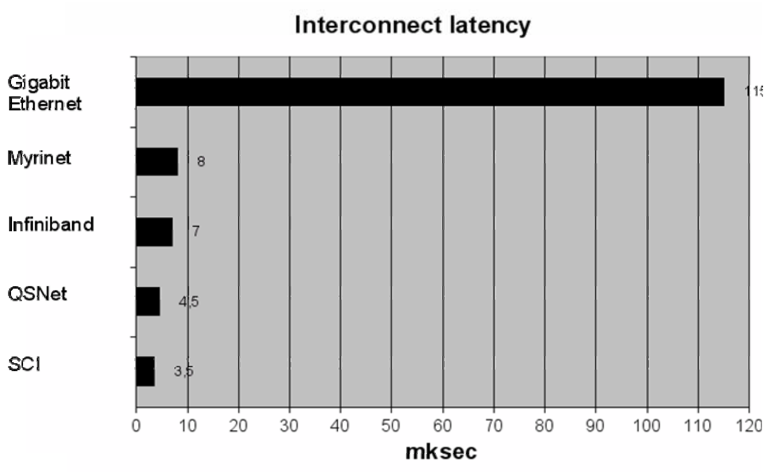
After the analysis, we choose an Itanium2 solution as the best scaling and best price/performance solution for floating point calculation intensive applications. But we understood that the selection of a newest Itanium2 architecture could cause problems with available 32-bit applications porting. So, we decided to build two systems. For SCIT-1 - a 32xCPU system we choose Xeon 2.67GHz platform and for SCIT-2 - a 64xCPU system we choose Itanium2 1.4GHz platform as the best one in 64-bit floating-point performer. It was also taken into account good perspective of Itanium2 architecture and its ability to operate faster with big precision operations and big memory. The other valued characteristics that cause better price/performance ratio of an Itanium2 systems is its best power/performance ratio between other well known general usage processors.



Picture 3. Interconnect throughput.

Design and a selection of internode communicational interfaces was done from the best performing ones. When making experiments with one of the software packages (Gromacs), we have found that a low latency is the most important issue for cluster scalability. We have seen from world published data and our own experiments that some of the tasks which don't scale more then 2-4 nodes on Gigabit Ethernet scales easily to 16 nodes on low-latency interconnect interfaces [3].

Understanding an importance of latency and throughput of an interface, we have made a price/performance analysis for interfaces available in Ukraine. The best one for 16x and 32x nodes' clusters we planned to build was SCI (Scalable Coherent Interface). Performance parameters of communicational interface received on 3rd quarter of the year 2004 for Intel Xeon platforms are shown on Picture 3 and Picture 4.



Picture 4. Interconnect latency

Today these pictures will look different (because of changes in platforms and interfaces itself), but price/performance leaders for latency intensive applications are SCI and QSNetII; for throughput intensive applications they are QSNetII and Infiniband. For small clusters an SCI is a preferable interface. But it has also one more useful feature. An SCI system network can be built on 2D mash topologies. Such architecture gives an ability to transfer data into two ways simultaneously. But to receive an advantage from this technology, software should be written with an understanding of this ability.

It is known that performance and intelligence are the most important factors promoting the development of modern universal high-performance computers. The first factor forced a development of parallel architectures. The rational base of this development is universal microprocessors, connected into cluster system architectures. The second factor becomes clear when the notion of machine intellect (MI) is used. The concept of MI is introduced by V.M.Glushkov. MI defines “internal computer intelligence” and the term “intellectualisation” is used to define an increase of machine intellect. During the last 5-6 years, V.M.Glushkov Institute of Cybernetics NAS of Ukraine carries out the research aimed at the development of cluster based, knowledge-oriented architectures called *intelligent solving machines* (ISM). ISM implementing high- and super-high-level languages (HLL and SHLL) and effective operation with large-size data- and knowledge bases. They operate as with traditional computation tasks (mathematical physics, modeling of complex objects and processes, etc.) as artificial intelligence (AI) tasks (knowledge engineering, pattern recognition, diagnosis, forecasting) [4].

Large-size complex data- and knowledge bases in these clusters are displayed as oriented graphs of an arbitrary complexity – trees, semantic networks, time constrained, etc. In ISM computers it is possible to build graphs with millions nodes and to represent various knowledge domains. It is also important that the developed architecture can be easily integrated with distributed database architectures, which are developed in Glushkov Institute of Cybernetics NAS Ukraine. This database architecture makes search processes and data processing much faster than solutions with traditional architectures.

The intellectual part of the cluster systems developed together with distributed databases is an advantage of this solution as compared with the systems developed in the other sites of the world.

Hardware and software of the systems developed. Today the following SCIT (supercomputer for informational technologies) supercomputers are built in the institute (Picture 5):

Picture 5. Photo of SCIT clusters.

SCIT-1 – 32xCPU, 16xNodes cluster on the basis of Intel Xeon 2.67GHz 32-bit processors. They are oriented to operate with 64-bit and 128-bit data. The peak performance of SCIT-1 is 170 GFlops with an ability to be upgraded to 0,5-1 TFlops (right on a photo).

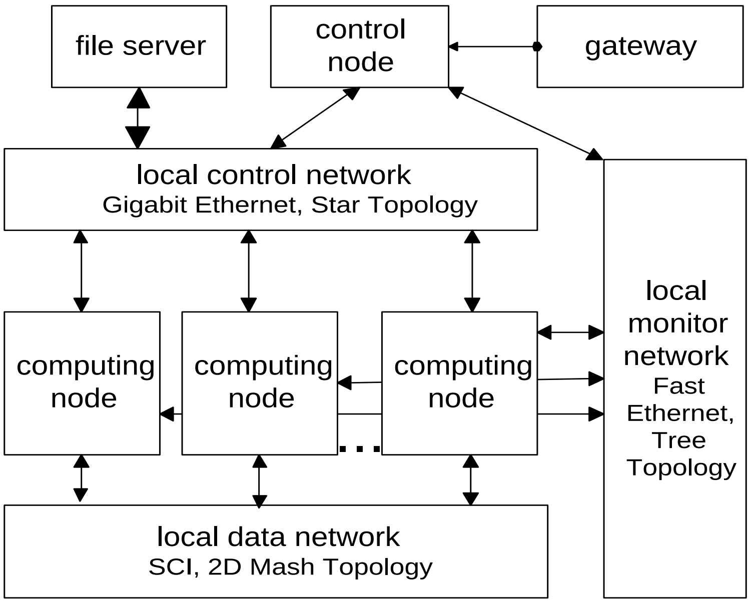
SCIT-2 – 64xCPU, 32xNodes cluster on the basis of Intel Itanium2 1.4GHz 64-bit processors. They are oriented to operate with 128-bit and 256-bit data. The peak performance of SCIT-2 is 358 GFlops with an ability to be upgraded to 2,0-2,5 TFlops. The storage system has capacity of 1 TByte and ability to be upgraded to 10-15 TBytes (left on the photo).

Each of two clusters is an array of computing nodes, connected together with three networks. The first one is a system network, based on SCI interface. The second one is a file data network, based on Gigabit Ethernet interface. The third one is a management network, based on Fast Ethernet interface. A general block-scheme of the SCIT supercomputer is shown on the Picture 6.

A local data network is based on SCI and is used for a high-performance low-latency inter-node communication during a calculation process. A local data network is built as 2D mash. For 16x node cluster it is configured as 4x4 or 2x8 2D mash. For 32x node cluster it is configured as 4x8 or 2x16 2D mash. On data transfers based on MPI the throughput for Xeon E7501 platforms is 250 MB/s, for Itanium2 8870 platforms – 355 MB/s.

A local control network is based on Gigabit Ethernet and is used to handle all cluster-computing nodes and to transfer data files between nodes and file server.

A local monitor network is used for service information transfer and monitoring of all the cluster system.



Picture 6. SCIT cluster structure.

On a table 1 performance parameters of SCIT-1 and SCIT-2 systems are described.

Performance characteristics of developed systems SCIT-1 and SCIT-2 are on the one stage with world best systems. They are also one of the best systems in a world mathematical supercomputing construction.

The creation of cluster systems SCIT-1 and SCIT-2 and their integration and finally launch was made due to a fruitful cooperation of Glushkov Institute of Cybernetics NAS of Ukraine with USTAR scientific and manufacturing company (based in Kiev) and Intel corporation (International). The partners of the institute delivered a technical support and consulting of a project.

Table 1. 64-bit performance parameters of SCIT-1 and SCIT-2 systems.

	SCIT-1	SCIT-2
1 Processors	P-IV Xeon 2,67 GHz	Itanium2 1,4 GHz
2 Peak performance of a single processor		
Integer operations per second, 10^9IPS	1,34	5,6
Floating point operations per second, GFLOPS	5,34	5,6
Node system bus performance, GB/s	4,2	6,4
3 Total peak performance of a system		
Integer operations per second, 10^9IPS	43	358
Floating point operations per second, GFLOPS	170	358
Total system bus performance, GB/s	67,2	204,8
4 Linpack performance of a system, GFLOPS	112,5	280

System Level Software

Components of system level software of a cluster support all stages of user-level parallel software development. They also provide execution of users processes of substantial processing on a solving field. They run on all the nodes of a cluster and a control node as well. Operating system used are ALT Linux for SCIT-1 and Red Hat Enterprise Linux AS for SCIT-2. Message Passing Interface (MPI) over SCI is used for programming in a message-passing model. In addition, system level software includes optimized compilers of C, C++, Fortran languages for parallel programming, fast Math libraries, etc.

Application Level Software

The powerful hardware, system level, service and specific cluster software integrated in a system is a strong ground for an application level software development. It gives an ability to solve new extra large tasks in a fields of science, economy, ecology, agriculture, technology, defense, space industry, etc.

Due to successful implementations of SCIT systems for the several months after the system was installed a lot of applications were developed and deployed on a supercomputer in Glushkov Institute of Cybernetics NAS of Ukraine.

The software packages for the following tasks were developed:

- soil ecology problems solution;
- seismic data processing;
- dynamical travelling salesman in a real time;
- modeling a structural-technological changes in a developing economy;
- a search for an optimal service center placement;
- construction of an interference-tolerant code;
- risk classification and evaluation decisions;
- data clusterization with genetics algorithms;
- decomposition, calculation, verification and solving of a theorems;
- software component for linear algebra;
- low-energy orbit selection;
- software package for a natural and technogenic processes analysis.

Conclusion

The supercomputer cluster project, as a first stage of a national supercomputer resources development, made a great impact on an intellectualisation of information technologies in Ukraine. The next stage will be devoted to improvement of performance characteristics of supercomputers designed and their software. This should allow extending an amount of large complex tasks that would be solved on the systems.

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Authors' Information

Valeriy N. Koval – Institute of Cybernetics NAS Ukraine; Prospekt Academika Glushkova,40, Kiev, 03680 MCP, Ukraine; e-mail: icdepval@ln.ua

Sergey G. Ryabchun – Institute of Cybernetics NAS Ukraine; Prospekt Academika Glushkova,40, Kiev, 03680 MCP, Ukraine; e-mail: sr@emt.com.ua

Volodymyr V. Savyak – Institute of Cybernetics NAS Ukraine; Prospekt Academika Glushkova,40, Kiev, 03680 MCP, Ukraine; e-mail: Volodymyr.Savyak@ustar.kiev.ua

Ivan V. Sergienko – Institute of Cybernetics NAS Ukraine; Prospekt Academika Glushkova,40, Kiev, 03680 MCP, Ukraine

Anatoliy A. Yakuba – Institute of Cybernetics NAS Ukraine; Prospekt Academika Glushkova, 40, Kiev, 03680 MCP, Ukraine; e-mail: ayacuba@voliacable.com

NEW KNOWLEDGE OBTAINING IN STRUCTURAL-PREDICATE MODELS OF KNOWLEDGE

Valeriy Koval, Yuriy Kuk

Abstract: An effective mathematical method of new knowledge obtaining on the structure of complex objects with required properties is developed. The method comprehensively takes into account information on the properties and relations of primary objects, composing the complex objects. It is based on measurement of distances between the predicate groups with some interpretation of them. The optimal measure for measurement of these distances with the maximal discernibleness of different groups of predicates is constructed. The method is tested on solution of the problem of obtaining of new compound with electro-optical properties.

Keywords: New knowledge, Predicates, Complex objects, Primary objects, Maximal discernibleness.

ACM Classification Keywords: I.2.4 Artificial Intelligence: knowledge representation formalisms and methods.

Introduction

The present work deals with further development of methods of practical extraction of knowledge from experimental data. Its purpose is development of an effective mathematical method for obtaining of new knowledge on the structure of complex objects with certain properties. The work is focused on solution of an important applied problem - designing of structure of compounds with the needed properties.

In our previous works [1] - [2] in order to obtain new knowledge in form of production rules, a concept of variable predicate, able to accept a number of values - so-called predicate constants, predicates in the conventional sense